

Additional File 2 to Scoring Function to Predict Solubility Mutagenesis – Confusion Matrices

Ye Tian¹, Christopher Deutsch² and Bala Krishnamoorthy*¹

¹Department of Mathematics, Washington State University, Pullman, WA 99164, USA

²Department of Chemistry, Portland State University, Portland, OR 97207, USA.

Email: Ye Tian - ytian@math.wsu.edu; Christopher Deutsch - cdeutsch@pdx.edu; Bala Krishnamoorthy* - bkrishna@math.wsu.edu;

*Corresponding author

Table 1: Confusion Matrix for LP (LOOCV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	48/59	15/78
Predicted as "Decreased Solubility"	11/59	63/78

Table 2: Confusion Matrix for SVM (LOOCV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	39/59	20/78
Predicted as "Decreased Solubility"	20/59	58/78

Table 3: Confusion Matrix for Lasso (LOOCV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	20/59	2/78
Predicted as "Decreased Solubility"	39/59	76/78

Table 4: Confusion Matrix for LP (10 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	46/59	18/78
Predicted as "Decreased Solubility"	13/59	60/78

Table 5: Confusion Matrix for SVM (10 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	43/59	18/78
Predicted as "Decreased Solubility"	16/59	60/78

Table 6: Confusion Matrix for Lasso (10 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	20/59	1/78
Predicted as "Decreased Solubility"	39/59	77/78

Table 7: Confusion Matrix for LP (3 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	45/59	18/78
Predicted as "Decreased Solubility"	14/59	60/78

Table 8: Confusion Matrix for SVM (3 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	37/59	21/78
Predicted as "Decreased Solubility"	22/59	57/78

Table 9: Confusion Matrix for Lasso (3 folds CV)

	Experimental classification	
	Increased Solubility	Decreased Solubility
Predicted as "Increased Solubility"	22/59	2/78
Predicted as "Decreased Solubility"	37/59	76/78